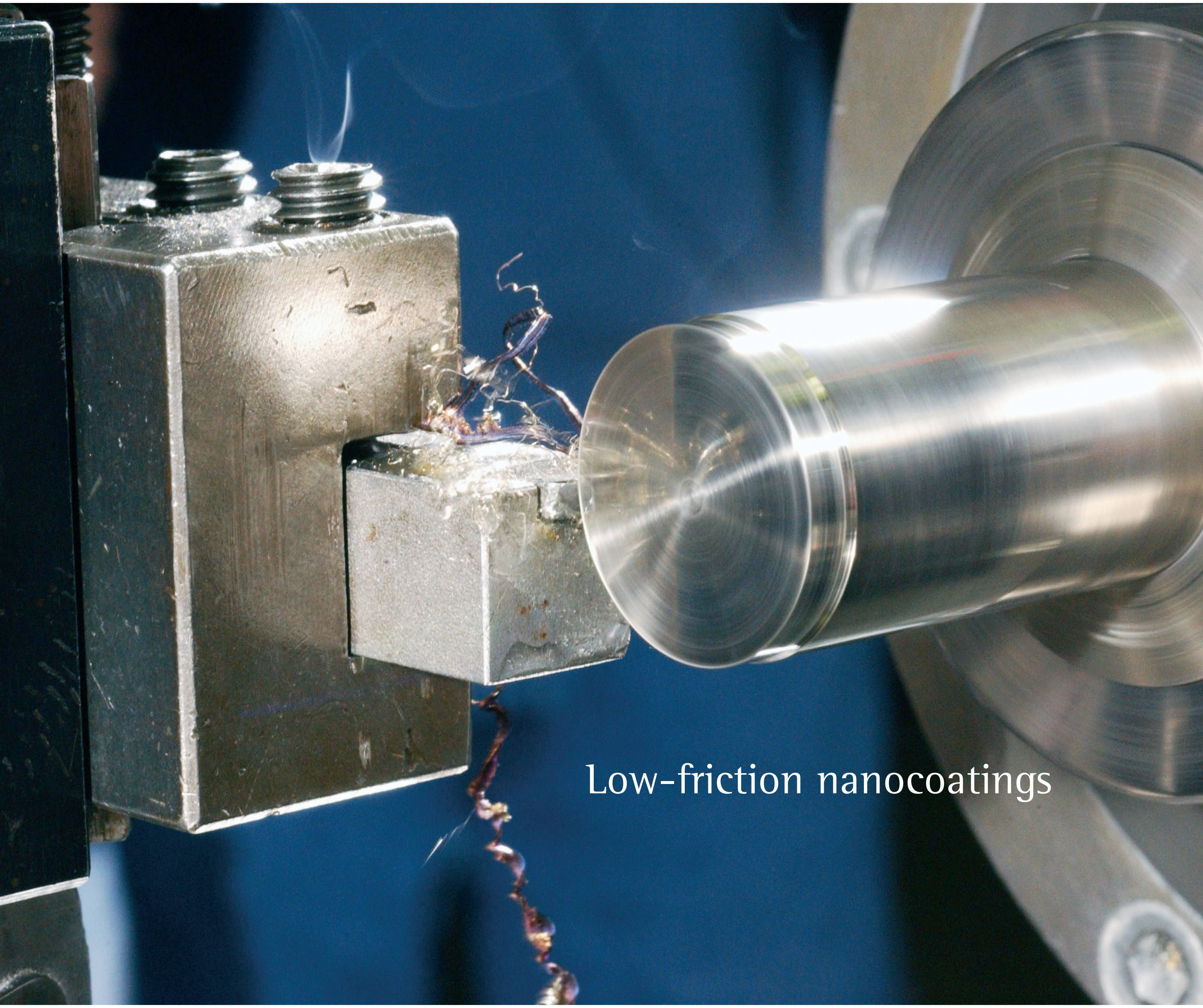
INQUIRY | FALL 2008

SCIENCE & TECHNOLOGY AT THE AMES LABORATORY



Low-friction nanocoatings

AMES LABORATORY
United States Department of Energy
Creating Materials and Energy Solutions

IOWA STATE UNIVERSITY

U.S. DEPARTMENT OF ENERGY

INQUIRY

Ames Laboratory is a U.S. Department of Energy laboratory seeking solutions to energy-related problems through the exploration of chemical, engineering, materials and mathematical sciences, and physics. Established in the 1940s with the successful development of the most efficient process to produce high-purity uranium metal for atomic energy, Ames Lab now pursues much broader priorities than the materials research that has given the Lab international credibility. Responding to issues of national concern, Ames Laboratory scientists are actively involved in innovative research, science education programs, the development of applied technologies and the quick transfer of such technologies to industry. Uniquely integrated within a university environment, the Lab stimulates creative thought and encourages scientific discovery, providing solutions to complex problems and educating tomorrow's scientific talent.

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For additional information about Ames Laboratory or topics covered in this publication, please contact:

Editor, *Inquiry*
Ames Laboratory
111 TASF
Ames, Iowa 50011-3020
515-294-9557
www.ameslab.gov

Inquiry is published biannually by the Ames Laboratory Office of Public Affairs. Iowa State University operates the Laboratory for the U.S. Department of Energy under contract DE AC02 07CH11358. Ames Laboratory shares a close working relationship with Iowa State University's Institute for Physical Research and Technology, a network of scientific research centers.

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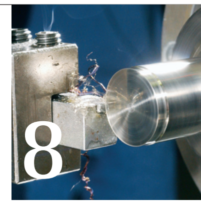
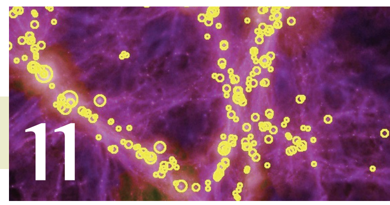
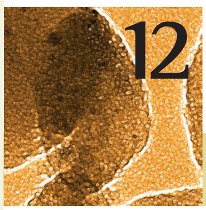
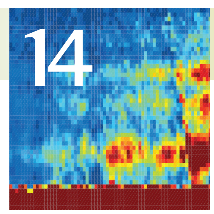
Contents



FEATURES







DEPARTMENTS

Cover: *A wafer of aluminum-magnesium-boride is used as machine tooling to make a heavy lathe cut in hardened stainless steel. Ames Laboratory researchers are studying use of the alloy, nicknamed BAM, as a coating for industrial applications with the goal of boosting energy efficiency of industrial equipment.*

From the Director

The Ames Laboratory has had a busy past few months. In the spring of this year, Chinese researchers announced the discovery of high-temperature superconductivity in a new pnictide compound based on iron and arsenic, and the scientific world was once again engaged in a race to replicate, extend and understand the results. Ames Lab researchers, led by Paul Canfield and working closely with our environmental safety and health professionals to ensure safe handling of these poisonous materials, were able to reproduce the results within days. A number of significant "firsts" ensued: we created new compounds that also demonstrated elevated-temperature superconductivity, building on the availability of rare earth elements from our Materials Preparation Center; among these was the first non-oxide, all-metallic superconducting FeAs compound; we created the first single crystal specimens suitable for making critical measurements, such as the phonon dispersion curves; and direct comparisons have been made between advanced theoretical and experimental work. Along the way, Rob McQueeney and his collaborators collected the first research results from the Wide Angular Range Chopper Spectrometer (ARCS) at Oak Ridge National Lab's new Spallation Neutron Source. The science is still emerging at a fast pace, and as I write 22 papers have been submitted to the physics archive server and submitted to archival journals, and 7 of them are already accepted for publication or in print. You will be able to read more about this in a future issue of *Inquiry*, after the dust settles a little.

Welcome to the Fall 2008 issue of Inquiry *magazine*

This summer's pnictide activity provides some striking examples of the capabilities, values and working methods that make the Ames Laboratory a unique national resource. In the spring, I commissioned a committee to look at our "brand" and they came up with seven "core values" that describe the ways that we do our work. These are listed on page 16, but it is worth noting how several of them contributed to our efforts this summer. **Safety** is one of our core values and distinguishing features; without our established safety culture it would have been impossible to undertake work focusing on arsenic. **Agility** allowed the Ames Lab to move quickly and responsively to address the emerging scientific opportunities. Our **People** contributed individual skills, time and effort, which produced greater results through extensive **Collaboration** that extended across different sectors of the Ames Laboratory to our partner national labs and far beyond. More than 20 people have been involved in this work, at Ames and around the world, in a team that could only be created by a national laboratory. Throughout the effort, **Excellence** has been the hallmark, as reflected in the quality and prestige of the journals that are publishing this work.

Our values are not something that we decide to use or not use, and neither are they a directive from the executive office: they are part of the instinct and intuition that characterizes the Lab at every level, and they emerge naturally as it does its work. The pnictide efforts illustrate how well the branding committee described the Ames Lab and what it does: **Creating Materials and Energy Solutions**.

Alex King, Director

Shechtman Receives E-MRS Award

Ames Laboratory research scientist Dan Shechtman received the European Materials Research Society 25th Anniversary award.

The E-MRS award is the highest recognition conferred upon a materials scientist by the society, which is Europe's leading organization for the support and advancement of research in materials. The award consisted of a plaque, a medal and a cash grant of 5000 euro (about $7,800) sponsored by both E-MRS and Elsevier. Shechtman was formally recognized with the award at a ceremony and banquet held in Strasbourg, France on May 28.

Dan Shechtman

Shechtman, who is also a faculty member in the Department of Materials Science and Engineering at Iowa State University, was selected by the award committee in recognition of his essential contribution to the discovery of quasi-periodic crystals, also known as quasicrystals, in metallic alloys. In 1982, he discovered the icosahedral phase in a rapidly solidified aluminum transition metal alloy, which opened up the field of quasicrystals as an area of study in materials science.

Shechtman was recruited to the Ames Laboratory and Iowa State through a joint effort between Pat Thiel, Ames Laboratory division director for Science and Technology and quasicrystal expert, and Mufit Akinc, who was then chair of ISU's Department of Materials Science and Engineering. Shechtman joined the staff at Ames Laboratory in 2004.

Harmon, Finnemore Outstanding Referees

Three Ames Laboratory scientists were recognized for their exceptional efforts in assessing manuscripts for American Physical Society journals. Doug Finnemore, senior physicist; Bruce Harmon, deputy Lab director and senior physicist; and a third physicist who requested to remain anonymous are in the inaugural group of Outstanding Referee award winners.

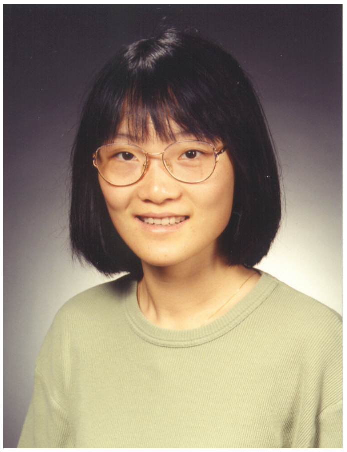
APS initiated the Outstanding Referee award this year to express appreciation to all referees whose efforts in peer review both maintain the high standards of APS journals and help authors improve the quality and readability of their articles.

"Manuscript reviewers often operate in the background without much recognition, but their contributions to their fields of research are enormously important," says Alex King, Ames Laboratory director. "We are pleased that three Ames Lab scientists have been recognized for their service."

Hong Receives "Young Chemist" Award

Ames Laboratory chemist Mei Hong was honored as a recipient of the Agnes Fay Morgan Award by the Iota Sigma Pi Honor Society for Women in Chemistry during the organization's 29th Triennial Convention June 26-29 in Cincinnati, Ohio.

The Morgan Award is presented annually to a woman age 40 or under in the field of chemistry or biochemistry and consists of $500, a certificate and membership in Iota Sigma Pi with a waiver of dues for one year. Hong was chosen for the award in 2006, but because the society formally meets only every third year, she was among the three award recipients recognized at this year's convention.



Mei Hong

Thiel Named Iota Sigma Pi Honorary Member

Pat Thiel

Pat Thiel, Ames Laboratory division director for Science and Technology, received the 2008 Iota Sigma Pi Honorary Member award from the National Honor Society for Women in Chemistry on June 27 at the organization's 29th Triennial Convention in Cincinnati, Ohio. Thiel is the 33rd recipient of the award, which was established in 1921 and has gone to three Nobel Laureates, including Marie Curie.

"This is a very distinguished recognition," says Ames Laboratory Director Alex King. "Iota Sigma Pi bestows only one honorary membership every three years, so it is very selective indeed. Pat has been a consistent pioneer in the field of chemistry and certainly deserves the honor. Ames Lab is proud to have her among its leaders."

NSF Early Career Award to Travesset

Alex Travesset, an associate scientist at Ames Laboratory, has received a National Science Foundation CAREER award, the organization's most prestigious award for junior researchers.

The NSF CAREER award recognizes researchers who exemplify the role of teacher-scholars through outstanding research, excellent education and the integration of education and research. The five-year, $410,000 award will support Travesset's theoretical study of the interaction of phospholipids, the molecules that form cell membranes, with GTPases, certain proteins that regulate signaling in cells.

Alex Travesset

Akinc Named ASM Fellow

Mufit Akinc, an associate scientist at Ames Laboratory, was elected a Fellow of ASM International, a society for materials scientists and engineers. Akinc was one of 19 ASM Fellows elected in 2008.

Akinc, who is also an Iowa State University professor of materials science and engineering, was honored for his "contributions to the science and technology of ceramics and alloy powders and for leadership in materials education."

Mufit Akinc

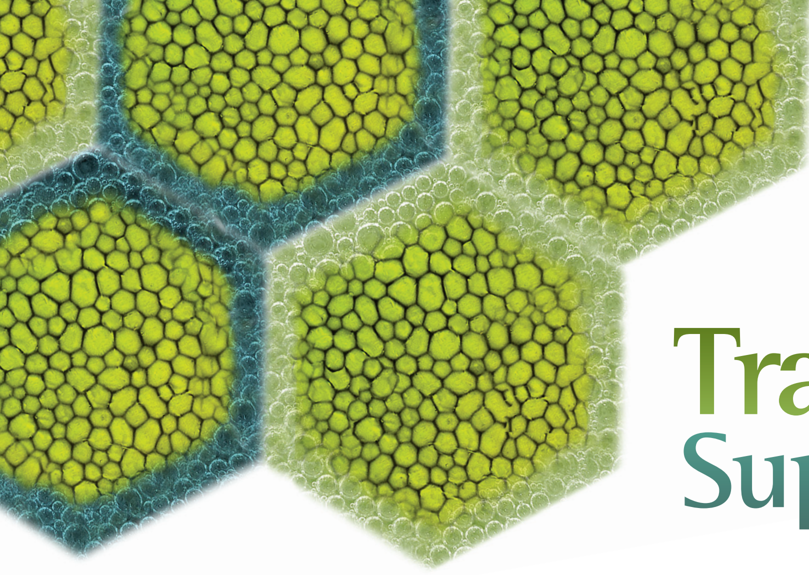
The Fellow designation was established by ASM International to provide recognition to members for their distinguished contributions to the materials science and engineering field. Fellows are considered technical and professional leaders who serve as advisors to the society, and they are selected by their peers in the organization.

MFRC Receives Tech Transfer Award

Ames Laboratory's Midwest Forensics Resource Center received the Outstanding Partnership award from the Federal Laboratory Consortium for Technology Transfer Mid-Continent Region. The FLC Outstanding Partnership award recognizes the MFRC's efforts to promote technology transfer between federal government facilities and the private or public sectors.

The MFRC develops new techniques in forensic science and transfers those techniques to crime laboratories throughout the Midwest. One method of technology transfer is collaborative crime lab-centered forensic research projects that partner crime laboratories with scientists at the MFRC or Midwestern universities.

"All of the MFRC's efforts are designed to develop, test and evaluate more efficient and reliable methods of analyzing evidence and to get information about those methods out into crime laboratories where we hope the new techniques will help busy forensic scientists," says David Baldwin, director of the MFRC. "We are pleased that the Federal Laboratory Consortium recognized our efforts and the efforts of our partner crime laboratories."



BY BREEHAN GERLEMAN LUCCHESI

Tracing the Image of Superconductivity

SUPERCONDUCTIVITY. EXPERIMENTATION. Analysis. Andrew Fidler learned a lot about all of these during his internship at Ames Laboratory. But he also learned that sometimes it takes some old-fashioned materials and techniques to make some brand new discoveries. Fidler, a 2007 participant in the Department of Energy's Science Undergraduate Laboratory Internship, or SULI, program, contributed to the groundbreaking discovery that the bubble-like arrangement of magnetic domains in superconducting lead exhibits patterns very similar to conventional froths. And Fidler's work was done with an office supply of the past: carbon paper.

Fidler used the carbon paper to gather the data Ames Lab physicist Ruslan Prozorov needed to analyze the polygon cells that make up the superconducting froths, called suprafroths. The process started with images of suprafroths taken with a magneto-optic microscope in Prozorov's lab that showed rough outlines of the froth's cells. Fidler's task was to take a pen and a piece of carbon paper and trace the microscope image to produce a clear picture of the polygons.

"In order to compare the suprafroths with conventional froths, we needed to identify the types and the amount of the polygons in each microscope image of the froth," says Prozorov. "We tried using computer programs to do it, but they failed. The images are very complex with gradients of intensity and some scratches and artifacts. There was no other way to do what Andrew did visually and manually, starting with the carbon paper."

"I actually had a hard time finding carbon paper," adds Prozorov. "I went to an office supply store, and they had to dig it out of the storage room somewhere."

Fidler traced each image by hand — twice.

"I traced once with carbon paper and once with black pen to make sure the lines would be read by the scanner, and then I scanned each tracing into the computer. I looked at the froth images on the computer screen and identified each type of polygon cell. Then I tabulated how many of each type of polygon was in each image," says Fidler.

Each image consisted of approximately 200-300 polygon cells, and Fidler repeated the process on 528 images, with each image representing a different point of temperature and magnetic field.

"It was a tremendous amount of work," says Prozorov.

Fidler and Prozorov's efforts — combined with the contributions of Ames Lab physicist Paul Canfield and Iowa State University graduate student Jake Hoberg — paid off. The group published their findings in *Nature Physics* in April 2008. Their paper proposed suprafroths as a model system for all froths.

"There are certain statistical laws that govern the behavior of froths, and we found that suprafroths satisfy these laws," says Prozorov. "We can now apply what we know of suprafroths to all other froths and complex froth-like systems."

Suprafroths offer reversibility, a significant benefit over conventional froths.

"In everyday froths, like soap foam, the agent of change is time," says Prozorov. "You have to wait for bubbles to simply dry out, and that takes days. And it's not reversible. You cannot reverse time."

But achieving an ideal froth experiment is possible with suprafroths because the agents that create the superconducting phase cells are magnetic field and temperature, both reversible parameters.

"Magnetic field and temperature can be tuned in the lab," says Prozorov. "They can be increased or decreased, and therefore we are able to study the pure statistical properties of froth without problems associated with the irreversibility of time or with chemical property changes."

Prozorov's comparison of suprafroths is also an important contribution to the study of superconductors.

"The statistical analysis shows suprafroths behave just like normal froth, which is also new for superconductivity," says Prozorov. "Just last year we found this new pattern in superconductors, and now we've proven that the froth state is really an intrinsic property of superconducting lead. It's a big deal for both the general physics of froth and the growing physics of superconductors."

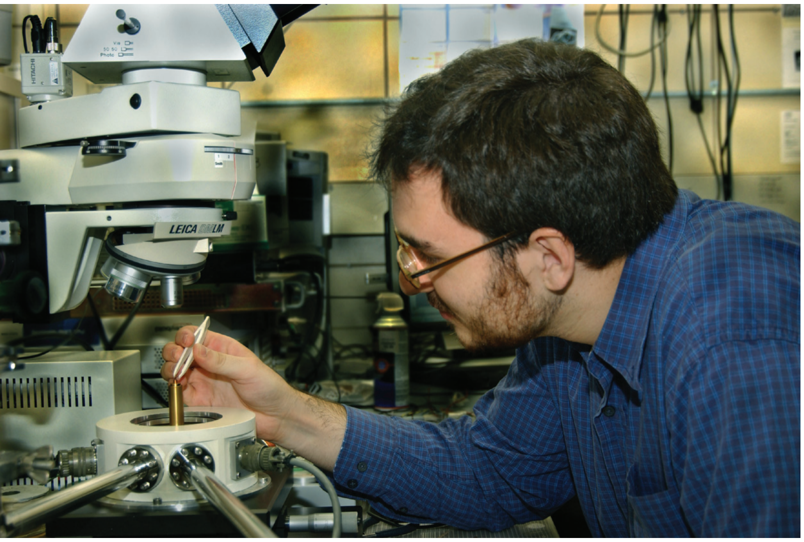
Fidler wasn't expecting to be involved with such a "big deal" when he applied for the SULI program.

"I was never expecting to be able to get a journal article published, let alone in such a reputable journal as *Nature Physics*," says Fidler. "I still don't think I have fully realized how significant it is to be published in such a good journal as an undergraduate. I'm really thrilled to be a published author.

"I learned so much working with Dr. Prozorov and his graduate students," adds Fidler. "Dr. Prozorov was always available to help, and the students in his lab explained everything I had questions about."

Following his internship at Ames Lab, Fidler nominated Prozorov for a SULI Outstanding Mentor award.

Fidler's nomination reads, in part, "Since my first day at Ames Laboratory, Dr. Prozorov has given me the opportunity to work on a challenging and interesting project,



Andrew Fidler prepares a sample for study in the low-temperature magnetism laboratory.

and he has provided insights and has been an effective instructional coach during my internship."

The next stop for Fidler is graduate study in physics at the University of Chicago.

"SULI definitely helped me attain my goal of attending graduate school," says Fidler, "and it validated my continued interest in the sciences, too."

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suprafroth \ `sü-prä `froth \ **n**
pl. **suprafroths** \ `sü-prä `froths, frothz

A Supra New Science Term

Why are Ruslan Prozorov's *super*conducting froths called *supra*froths? The term was born of necessity but is based on history.

"Originally we wanted to call the new froth 'superfroth' simply because of the term 'superconductor,'" says Prozorov. "But if you do a Web search for superfroth, you see the term is already taken by some totally unrelated materials like plastics, milk for coffee drinks and even ice. And the term superfroth is even trademarked by one company."

"So we invented the term 'suprafroth' to avoid any trademark troubles and because when superconductors were first invented they were called 'supraconductors,'" Prozorov continues. "Well, the term was originally in German, but as the science of what is now called 'superconductors' spread across Europe, they were most often called supraconductors."

"Many people like the term suprafroth now, and the term is clearly distinct," he adds. "A Google search gives only results for what we have come up with. And while the term is already propagating through the scientific community, all references to the work will point back to our work. It's not really often you can coin a term, but we managed to do just that."

Nano, Tough and Super Slick

A nanoscale coating of an aluminum-magnesium-boride helps reduce friction and boosts industrial energy efficiency

BY KERRY GIBSON

FRICTION IS THE BANE OF ANY MACHINE. When moving parts are subject to friction, it takes more energy to move them, the machine doesn't operate as efficiently, and the parts have a tendency to wear out over time.

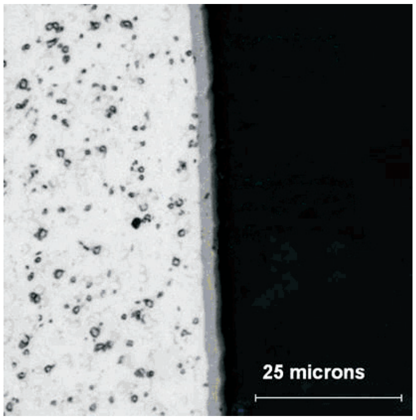
But if you could manufacture parts that had tough, "slippery" surfaces, there'd be less friction, requiring less input energy and the parts would last longer. Researchers at the Ames Laboratory are collaborating with other research labs, universities and industrial partners to develop just such a coating.

"If you consider a pump, like a water pump or a hydraulic pump, it has a turbine that moves the fluid," says Bruce Cook, an Ames Laboratory scientist and co-principal investigator on the four-year, $3 million project. "When the rotor spins, there's friction generated at the contacting surface between the vanes and the housing, or stator. This friction translates into additional torque needed to operate the pump, particularly at start-up. In addition, the friction results in a degradation of the surfaces, which reduces efficiency and the life of the pump. In other words, it takes extra energy to get the pump started, and you can't run it at its optimum (higher speed) efficiency because it would wear out more quickly."

Applying a coating to the blades that would reduce friction and increase wear resistance could have a significant effect in boosting the efficiency of pumps, which are used in all kinds of industrial and commercial applications. According to Cook, government calculations show that a modest increase in pump efficiency resulting from use of these nanocoatings could reduce U.S. industrial energy usage by 31 trillion BTUs annually by 2030, or a savings of $179 million a year.

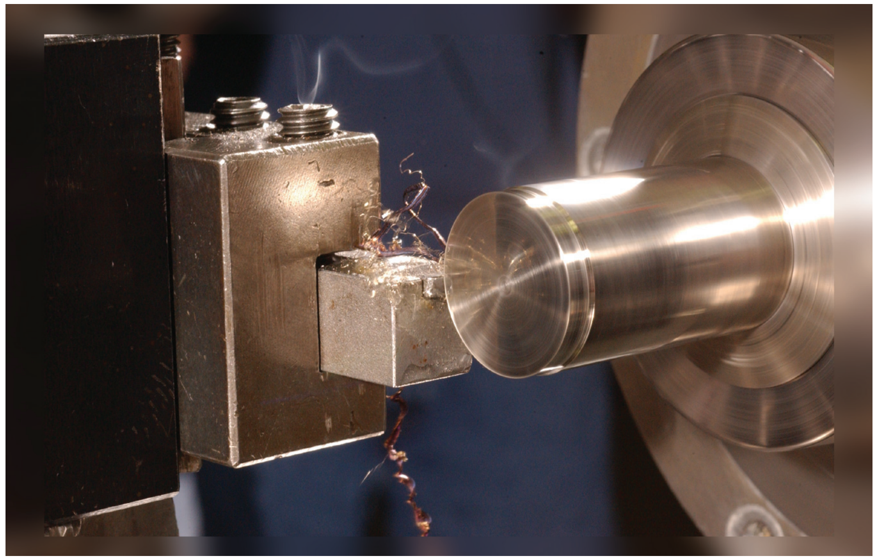
The coating Cook is investigating is a boron-aluminum-magnesium ceramic alloy he discovered with fellow Ames Laboratory researcher and Iowa State University professor of materials science and engineering Alan Russell about eight years ago. Nicknamed BAM, the material exhibited exceptional hardness and an even lower coefficient of friction than Teflon®. The research has expanded to include titanium-diboride alloys as well.

In many applications it is far more cost effective to apply the wear-resistant materials as a coating than to manufacture an entire part out of the ceramic. Fortunately, the BAM material is amenable to application as a hard, wear-resistant coating. Working with ISU materials scientist Alan Constant, the team is using a technique called pulsed laser deposition to deposit a thin layer of the alloy on hydraulic pump vanes and tungsten carbide cutting tools. Cook is working with Eaton Corporation, a leading manufacturer of fluid power equipment, using another, more commercial-scale technique known as magnetron sputtering to lay down a wear-resistant coating.



A photograph of an $AlMgB_{14}$ coating on a steel substrate. The coating is the thin, darker strip running along the edge of the steel. (The blemishes on the steel are carbide inclusions) The coating has a thickness of approximately 2 to 3 microns.

(Opposite) This image shows coating of a substrate (left) with $AlMgB_{14}$ by pulsed laser deposition. The bright plume in the center of the photograph is an $AlMgB_{14}$ plasma. The solid target is just to the right of the plume.



(Right) In an early test of BAM's capabilities, a sharpened wafer of the material is used as machine tooling to make an heavy lathe cut in hardened stainless steel.

Pumps aren't the only applications for the boride nanocoatings. The group is also working with Greenleaf Corporation, a leading industrial cutting tool maker, to put a longer lasting coating on cutting tools. If a tool cuts with reduced friction, less applied force is needed, which directly translates to a reduction in the energy required for the machining operation.

To test the coatings, the project team includes Peter J. Blau and Jun Qu at one of the nation's leading friction and wear research facilities at the U.S. Department of Energy's Oak Ridge National Laboratory, or ORNL, in Tennessee. Initial tests show a decrease in friction relative to an uncoated surface of at least an order of magnitude with the $AlMgB_{14}$-based coating. In preliminary tests, the coating also appears to outperform other coatings, such as diamond-like carbon and TiB_2.

In a separate, but somewhat related project, Cook is working with researchers from ORNL, Missouri University of Science and Technology, the University of Alberta, and private companies to develop coatings in high-pressure water jet cutting tools and severe service valves where parts are subject to abrasives and other extreme conditions. The water jets use a slurry containing abrasive grit that's forced through nozzles at 60,000 to 87,000 pounds per square inch and can make intricate cuts in almost any material without the risk of heat warpage. Unfortunately the abrasive also wears out the nozzles and the hope is that a coating of BAM can extend nozzle life.

"This is a great example of developing advanced materials with a direct correlation to saving energy," Cook says. "Though the original discovery wasn't by design, we've done a great deal of basic research in trying to figure out the molecular structure of these materials, what gives them these properties and how we can use this information to develop other, similar materials."

According to Russell, BAM isn't like most superhard materials, such as diamond, that have a simple, regular and symmetrical crystalline structure. Instead, BAM's structure is complex, unsymmetrical, and its lattice contains gaps. As for its slipperiness, Russell speculates that boron oxidation takes place on the surface and these tiny amounts of boron oxide attract water molecules from the air, to make the coating slippery.

"It's almost as if it's a self-lubricating surface," he says. "It's inherently slippery so you don't need to add oil or other lubricants."

While Cook and Russell continue their research, efforts are also underway to bring the material to the market commercially. BAM is licensed to Newtech Ceramics, an Iowa based startup company located in Des Moines. The ISU Research Foundation provided nearly $60,000 in funding for development of material samples for marketing as part of the startup effort.

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For more information:
Bruce Cook, (515) 294-9673
cook@ameslab.gov

Research funded by:
DOE Office of Energy Efficiency and Renewable Energy

BY SAREN JOHNSTON

Filtering out the Noise

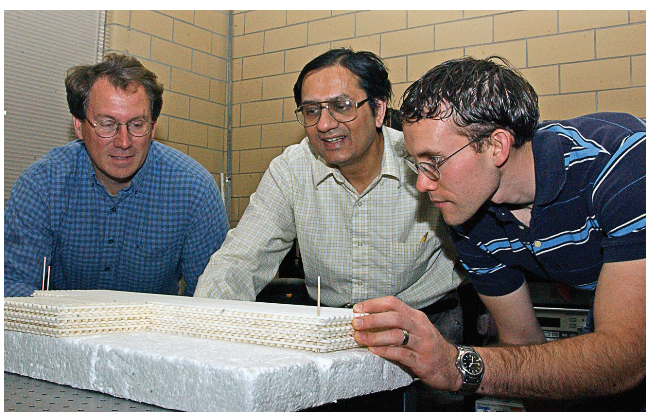
3-D photonic crystals help clear up fiber optic data transmission

Ames Laboratory researchers have come up with a potentially perfect way to sort and distribute the massive amounts of data that travel daily over optical fibers to people throughout the world. The new technology, a three-dimensional photonic crystal add-drop filter, promises greatly enhanced transmission of multiple wavelength channels (wavelengths of light) traveling along the same optical fiber.

The innovative filter is a significant achievement in the effort to develop all-optical transport networks that would eliminate electrical components from optical transmission links and guarantee virtually flawless data reception to end users of the Internet and other fiber-based telecommunications systems.

"There are up to 160 wavelength channels traveling through an optical fiber at the same time," says Rana Biswas, physicist and one of the developers of the new add-drop filter. "That means a lot of dialogue is going on simultaneously."

Biswas, who is also an Iowa State University adjunct associate professor of physics and astronomy and electrical



Researchers (from left) Gary Tuttle, Rana Biswas and graduate student Dan Stieler examine defects in a photonic crystal.

and computer engineering, explains that as information is transported over multiple channels, it's necessary to drop off individual wavelength channels at different points on the fiber. At the same time, it's essential to be able to add data streams into unfilled wavelength channels.

"When the data being transported in multiple frequency channels over an optical fiber comes to a receiving station, you want to be able to pick off just one of those frequencies and send it to an individual end user," says Biswas. "That's where these 3-D photonic crystals come into play."

Biswas and his colleagues, Kai-Ming Ho, senior physicist and an ISU Distinguished Professor of Liberal Arts and Sciences; Gary Tuttle, an ISU associate professor of electrical and computer engineering and a researcher at the university's Microelectronics Research Center; and Preeti Kohli, a former Iowa State Ph.D. student now at Micron in Manassas, Va. successfully demonstrated that 3-D photonic crystals could serve as add-drop filters, providing greatly enhanced data transmission.

To prove their concept, the researchers used a three-dimensional, microwave-scale photonic crystal constructed from layered alumina rods and containing a full bandgap – a wavelength range in which electromagnetic waves cannot transmit. Just as electronic bandgaps prevent electrons within a certain energy range from passing through a semiconductor, photonic crystals create photonic bandgaps that confine light of certain wavelengths.

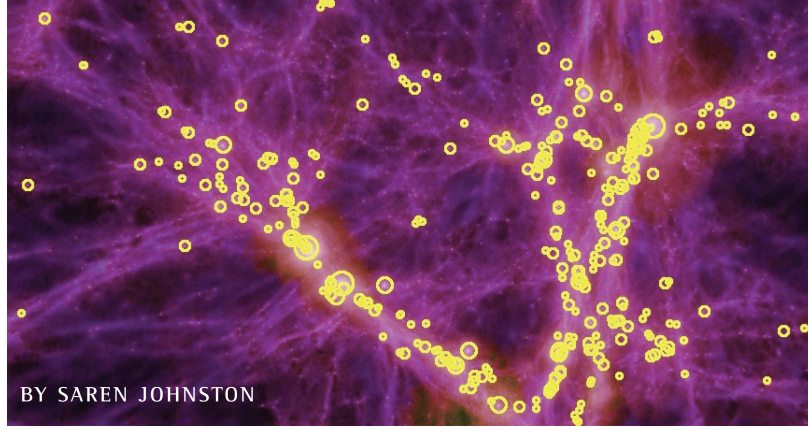
Although the team has shown that 3-D photonic crystals would make highly efficient add-drop filters, there are still problems to address. Getting the size of the photonic crystals down to work at the wavelengths used for Internet communications – 1.5 microns – is the big challenge. The group now has some of these photonic crystals working in that range, but to make these controlled structures with one input, another output and a defect … that definitely takes some work. A future direction is to simplify the design of the add-drop filter by reducing the layers in the photonic crystal – perhaps having all the action happen in one layer.

For more information:
Rana Biswas, (515) 294-6987
biswasr@ameslab.gov

Research funded by:
DOE Office of Basic Energy Sciences

Spinning Toward Reality

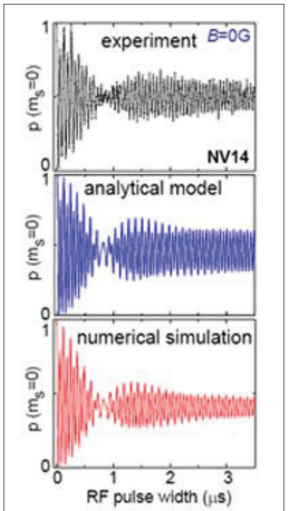
Quantum computing takes a step forward



BY SAREN JOHNSTON

RESEARCHERS AT AMES LABORATORY; The University of California, Santa Barbara; and Microsoft Station Q have teamed up to learn how quantum-mechanical states break down. The scientists made significant advancements in understanding one of the fundamental problems of quantum mechanics, which is also blocking efforts to develop practical quantum computers: the problem of decoherence. Their respective theoretical and experimental studies investigate how a single microscopic object loses its quantum-mechanical properties through interactions with the environment.

"Quantum-mechanical particles can interact with their environments: visible light, or photons; molecules of the air; crystal vibrations; and many other things," says Viatcheslav Dobrovitski, an Ames Laboratory theoretical physicist. "All these uncontrollable interactions randomly 'kick' the system, destroying quantum phases, or the ability of particles to preserve coherence between different quantum states."



These images depicting coherently driven spin oscillations of a nitrogen-vacancy (N-V) center show the excellent level of agreement achieved between experiment, analytical theory and computer simulation.

Quantum coherence is essential to developing quantum computers in which information would be stored and processed on quantum mechanical states of quantum bits, called qubits. So the self-destructive nature of quantum-mechanical states interacting with the environment is a huge problem.

To find out more about how quantum coherence breaks down and to study the dynamics of this decoherence process, the Ames Lab, UCSB and Microsoft Station Q team studied certain spin systems called nitrogen-vacancy, N-V, impurity centers in diamond. The researchers were able to manipulate a single N-V center interacting with an environment of nitrogen spins in a piece of diamond. Amazingly, they were able to tune and adjust the environmental interference extremely well, accessing surprisingly different regimes of decoherence in a single system. They showed that the degree of interaction between the qubit and the interfering environment could be regulated by applying a moderate magnetic field. By using analytical theory and advanced computer simulations, the scientists gained a clear qualitative picture of the decoherence process in different regimes, and also provided an excellent quantitative description of the quantum spin dynamics. The experiments were performed at room temperature rather than at the extremely low temperatures often required for most atomic-scale investigations.

Dobrovitski notes that quantum coherence of N-V centers in diamond is being studied by leading scientific groups worldwide. "The combined efforts of these groups could help in opening the way to developing a series of interacting qubits – steps to a quantum computer – where each N-V center would act as a qubit," he says.

"In addition to quantum computers, quantum coherence plays an important role for future less exotic, but not less spectacular, applications," says Dobrovitski. For instance, quantum spins can be employed to develop coherent spintronic devices, which would work much faster than traditional microelectronic elements and dissipate much less energy. Quantum coherence between many spins can be employed to drastically increase the sensitivity of modern nuclear magnetic resonance, NMR, or electron spin resonance, ESR, experiments," he adds. "From the application point of view, it is important to understand the loss of coherence of quantum systems in solid-state environments, which form the basis of modern technology."

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Note: This research was selected as the basis for the cover of the April 18, 2008 issue of Science *magazine -- http://www.sciencemag.org/content/vol320/issue5874/cover.dtl A professional article about the research appears on pages 352-355.*

For more information:
Viatcheslav Dobrovitski, (515) 294-8666
slava@axel.ameslab.gov

Research funded by:
DOE Office of Basic Energy Sciences and the Air Force Office of Scientific Research Machines Program

"Garbage In, Ethanol Out"

BY KERRY GIBSON

New catalyst and old technology combine to turn waste material into biofuel

SAY THE WORD "BIOFUELS" AND MOST people think of grain ethanol and biodiesel. But there's another, older technology called gasification that's getting a new look from researchers at Ames Laboratory and Iowa State University. By combining gasification with high-tech nanoscale porous catalysts, they hope to create ethanol from a wide range of biomass, including distiller's grain left over from ethanol production, corn stover from the field, grass, wood pulp, animal waste and garbage.

Gasification is a process that turns carbon-based feedstocks under high temperature and pressure in an oxygen-controlled atmosphere into synthesis gas, or syngas. Syngas is made up primarily of carbon monoxide and hydrogen (more than 85 percent by volume) and smaller quantities of carbon dioxide and methane.

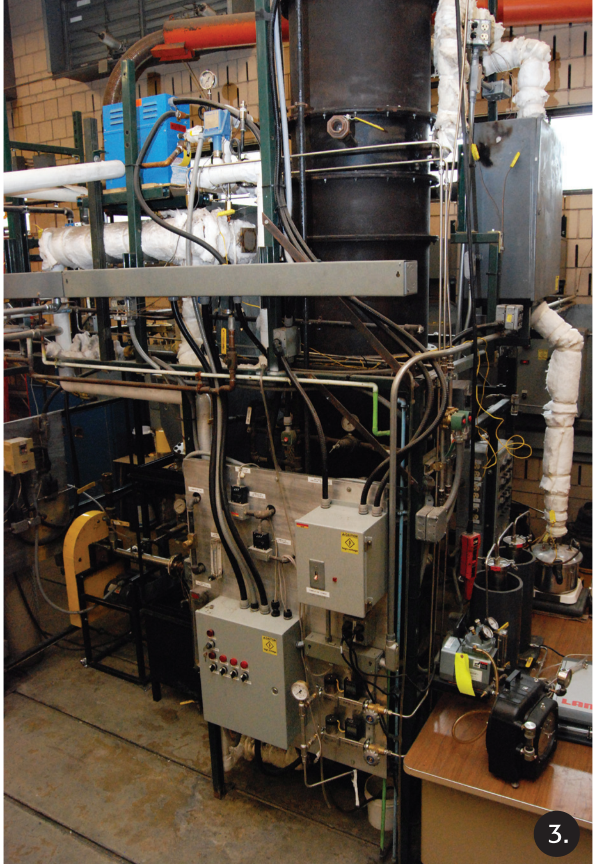
It's basically the same technique that was used to extract the gas from coal that fueled gas light fixtures prior to the advent of the electric light bulb. The advantage of gasification compared to fermentation technologies is that it can be used in a variety of applications, including process heat, electric power generation and synthesis of commodity chemicals and fuels.

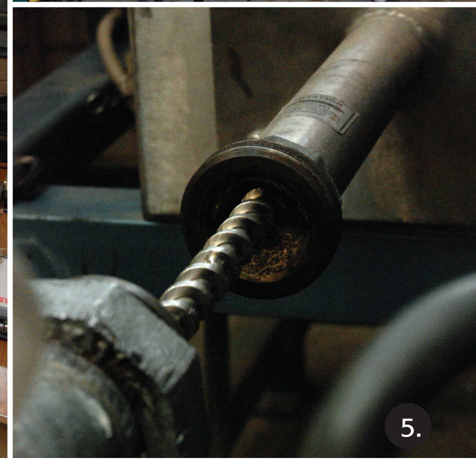
"There was some interest in converting syngas into ethanol during the first oil crisis back in the 70s," says Ames Lab chemist and Chemical and Biological Science Program Director Victor Lin. "The problem was that catalysis technology at that time didn't allow selectivity in the byproducts. They could produce ethanol, but you'd also get methane, aldehydes and a number of other undesirable products."

A catalyst is a material that facilitates and speeds up a chemical reaction without chemically changing the catalyst itself. In studying the chemical reactions in syngas conversion, Lin found that the carbon monoxide molecules that yielded ethanol could be "activated" in the presence of a catalyst with a unique structural feature.

"If we can increase this 'activated' CO adsorption on the surface of the catalyst, it improves the opportunity for the formation of ethanol molecules," Lin says. "And if we can increase the amount of surface area for the catalyst, we can increase the amount of ethanol produced."

Lin's group looked at using a metal alloy as the catalyst. To increase the surface area, they used nanoscale catalyst particles dispersed widely within the structure of mesoporous nanospheres, tiny sponge-like balls with thousands of channels running through them. The total surface area of these dispersed catalyst nanoparticles is roughly 100 times greater than the surface area you'd get with the same





1. *This micrograph shows mesoporous silica nanoparticles containing the catalyst particles (dark spots);* ***2.*** *Shredded corn stover is one of the test feedstocks;* ***3.*** *and* ***4.*** *The fluidized bed gasifier;* ***5.*** *Feedstocks are fed into the gasifiers by an auger.*

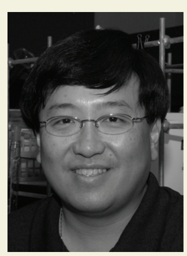
quantity of catalyst material in larger, macro-scale particles.

It is also important to control the chemical makeup of the syngas. Researchers at ISU's Center for Sustainable Environmental Technologies, or CSET, have spent several years developing fluidized bed gasifiers to provide reliable operation and high-quality syngas for applications ranging from replacing natural gas in grain ethanol plants to providing hydrogen for fuel cells.

In this process, a bed of sand is heated until it behaves like a fluid at about 1,350 degrees Fahrenheit. Feedstocks, such as switchgrass or corn stover, are pushed into the gasifier and when the material hits the bed of sand, it goes quickly from solid to gas, leaving only ash behind. The ash is separated from the gas stream and both the ash and syngas are collected. The ash, which contains nearly all of the nitrogen and phosphorous of the original crop residue, can be returned to the field so the soil is not depleted of those elements.

"Gasification to ethanol has received increasing attention as an attractive approach to reaching the national Renewable Fuel Standard of 36 billion gallons of biofuel," says Robert Brown, CSET director.

"The great thing about using syngas to produce ethanol is that it expands the kinds of materials that can be converted into fuels," Lin says. "You can use the waste product from the distilling process or any number of other sources of biomass, such as switchgrass or wood pulp. Basically any carbon-based material can be converted into syngas. And once we have syngas, we can turn that into ethanol."



For more information:
Victor Lin, (515) 294-3135
vsylin@iastate.edu

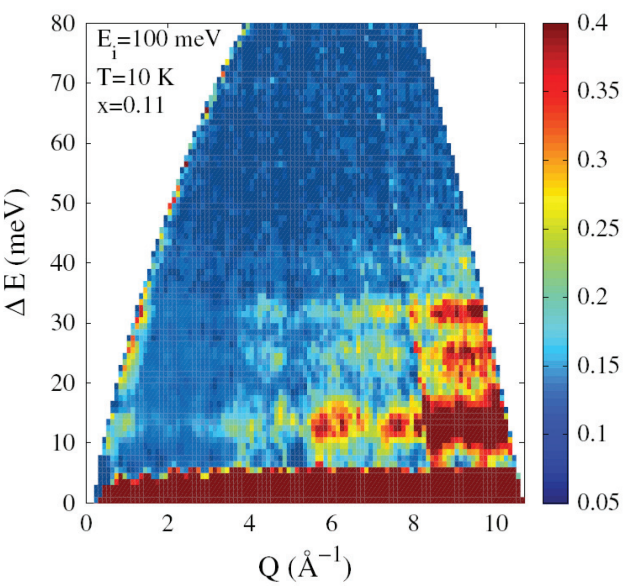
Research funded by:
DOE Office of Basic Energy Sciences and Energy Efficiency and Renewable Energy

A New Spin on Superconductivity

BY KERRY GIBSON

Using a new tool at the Spallation Neutron Source, researchers probe iron-arsenide materials

RESEARCHERS AT AMES LABORATORY ARE part of a collaborative team that's used a brand new instrument at the DOE's Spallation Neutron Source to probe iron-arsenic compounds, the "hottest" new find in the race to explain and develop superconducting materials. Rob McQueeney, an Ames Lab physicist, was part of that team whose findings, published in the Oct. 8 issue of *Physical Review Letters*, mark the first research produced with the aid of the new tool.



Inelastic neutron scattering intensity (color scale) of $LaFeAsO_{0.89}F_{0.11}$ (S2) at 10 Kelvin as a function of Q and E. The scattering due to the empty sample holder has been removed.

The Spallation Neutron Source – SNS for short – is the DOE's sprawling new $1.4 billion complex operated by Oak Ridge National Laboratory in the rolling green hills of eastern Tennessee. The SNS uses a pulsed neutron beam to provide information about the structure and dynamics of materials that cannot be obtained from X-rays or electron microscopes. Although neutral in electrical charge, neutrons interact with the nucleus. The neutron's magnetic moment can also interact with magnetic spins in a material. As neutrons from the beam pass through a material, they scatter off the nuclei and spins. By measuring the speed and angle of the scattered neutrons, scientists are able to develop detailed information about the positions and the motion of the nuclei and spins within the material.

McQueeney serves on the Executive Committee of the Instrumentation Development Team for ARCS, a wide angular-range chopper spectrometer designed to measure the vibrations of atomic nuclei. The sixth of the proposed 24 instruments to be built at the SNS, ARCS is undergoing final testing and is available for general use this fall, but McQueeney is already impressed with the results.

"The preliminary results are amazing," McQueeney says. "I have experience with a similar instrument and ARCS blew it away," adding that it produces better results from smaller samples in a much shorter time frame.

The timing of the testing phase for ARCS was ideal because in the preceding months, a new class of superconducting materials – pnictide compounds based on iron and arsenic – was discovered. This allowed McQueeney and collaborators at Oak Ridge National Laboratory and Cali-

The DOE's Spallation Neutron Source in Oak Ridge, Tenn., where McQueeney's neutron scattering research was conducted.

fornia Institute of Technology to look specifically at lanthanum-iron-arsenide ($LaFeAsO_{0.89}F_{0.11}$). One of the samples studied was produced by McQueeney's Ames Laboratory colleague, physicist and crystal-growth expert Paul Canfield. When this new class of superconductors was first announced, Canfield was able to quickly replicate the results and develop additional compounds.

The phenomenon of superconductivity is caused by the pairing of conduction electrons due to forces within the crystal. The origin of this pairing is one of the great unsolved mysteries in the field of high-temperature superconductivity.

"There are two prevailing ideas behind superconductivity," McQueeney says. "One is that pairing is mediated by lattice vibrations. The other is that it's mediated by magnetic or spin fluctuations."

Since neutrons are capable of measuring both the lattice vibrations and spin fluctuations, they are an ideal probe to gain an understanding of superconductivity.

The experiments focused on understanding the role of lattice vibrations in the new superconductors. The vibration of atoms within the crystal lattice creates a pattern of waves called phonons. When a neutron collides with this lattice, it can give up some of its energy to create a phonon. The difference in the neutron's energy before and after the collision is equal to the phonon energy.

"Our measurements did not support the conventional electron-phonon mediated superconductivity," McQueeney says, adding that theoretical calculations matched up fairly well with measurements obtained with ARCS. While the results are an important first step, there is still much work to be done to determine the origin of superconductivity in the iron-arsenides. McQueeney and his collaborators are continuing studies of phonons and spin excitations in these compounds.

The quest to understand and develop superconductor technology has important energy implications. By their nature, and as the name implies, superconductors can conduct electrical current with virtually no power loss, unlike conventional electric transmission lines that lose up to 30 percent due to resistance in the system. Basic research to understand the atomic interactions that make superconductors work, and to potentially control those properties, is one way that Ames Laboratory strives to address the scientific challenges facing our country.

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For more information:
Robert McQueeney, (515) 294-3545
mcqueeney@ameslab.gov

Research funded by:
DOE Office of Basic Energy Sciences

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Ames Laboratory
111 Technical and Administrative Services Facility
Ames, Iowa 50011-3020
515-294-9557
www.ameslab.gov

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